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Mathematical Simulation Models of Decomposition Processes

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SUMMARY

The general paradigm and its variants provide a useful framework for examining and comparing tundra decomposition models. The models themselves facilitate isolation of explicit and implicit constraints on theory which in turn helps to identify those areas requiring future development. The paradigm is not applicable to all decomposition models. Models incorporating microbial population dynamics (F. Bunnell, 1972; Whitfield, 1973; P. Bunnell, 1973) do not, in general, have the decomposition rate proportional to the amount of decomposing substrate . Only recently have sufficient data been available to provide estimates of the functional relationships influencing microbial population ecology.

The general microbial respiration model can be related to population dynamics. As it is offered here the respiration model represents an explicit framework within which various aspects of decomposition can be rigorously analyzed. All models should be "disposable." The models discussed in this paper should be retained only until they are replaced by a model or theory of stronger biological basis.
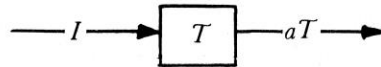
INTRODUCTION

The purpose of this paper is to present a "state of the art" discussion of mathematical simulation models as they have been applied to decomposition processes within the IBP Tundra Biome. We will do this by presenting a general paradigm applicable to most decomposition modeling which facilitates comparisons of the common features of the various models. The paradigm thus represents a model of models. We will use this paradigm to compare models arising within different national programs and to trace the historical development of modeling approaches within the US program where modeling approaches have been particularly diverse. We anticipate that this overview of modeling will provide some insights into what modeling is, how it has aided synthesis, and how it has evolved within the Tundra Biome.

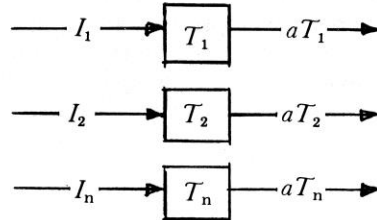# HISTORICAL OVERVIEW

The General Paradigm

The general paradigm is essentially that of Jenny, Gessel & Bingham (1949). Expressed in terms of a compartment model using discrete time steps it has the following form.
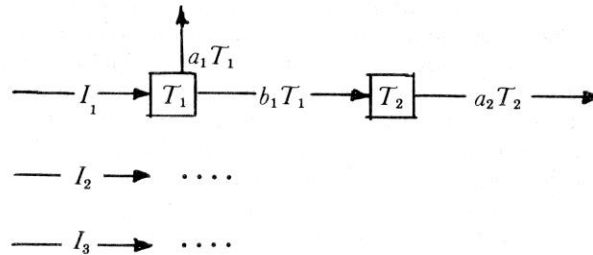
Example 1

At each iteration the total accumulated quantity of material under consideration, T, is incremented by an input I and decremented by an output proportional to T, $a \times T$. For example, I might be the yearly production of litter, T the total accumulated litter, and $a \times T$ the yearly loss of litter through respiration, leaching, and comminution. "Complex" or "complicated" models often simply consider a number of different types of material simultaneously. These types may be different plant species or woody and non-woody portions of the same plant species.

Example 2

The most "complicated" models have the output, or a fraction of the output, from one "compartment" serve as the input to one of the other compartments. In this form litter of varying ages (and perhaps different species) might be assumed representable by different compartments.

Example 3

$$I_1 \rightarrow \boxed{T_1} \quad \uparrow a_1 T_1 \quad - b_1 T_1 \rightarrow \boxed{T_2} \quad - a_2 T_2 \rightarrow$$

$$- I_2 \rightarrow \quad \cdots$$

$$- I_3 \rightarrow \quad \cdots$$

In their model of production and decay in a blanket bog at Moor House, UK, Jones & Gore (in press) incorporated both elaborations of the above paradigm. Their model can be viewed as a series of 1-cm-deep boxes representing sequential layers in the peat. The input of dead material is added to the top box and any overflow from a box is caught by the next successive box. Thus, they incorporate the elaboration of inter-connected boxes (example 3). Within each box, the peat is subdivided into six independently decomposing substrates: *Calluna* shoots, wood, and below-ground parts; *Eriophorum* leaves and below-ground parts; and *Sphagnum*. The separate treatment of different materials is analogous to the first elaboration of the paradigm (example 2). Each compartment loses weight or "decomposes" at a substrate specific decay rate modified by depth. This "depth modifier" is the same for all substrates and decreases the rate with depth.

The model of Clymo (in press) for peat bog growth is in some sense simpler than that of Jones & Gore. The model utilizes a number of depths or layers but does not subdivide the peat into a number of independent substrates; nor does the model utilize a different decay rate for each depth. The model hypothesizes two decay rates, one above the water table level representing aerobic decomposition, and one below the water table level representing anaerobic decomposition. The sophistication of Clymo's model lies in its handling of the physical processes of compaction and creep and its development of a complex differential equation.

The ABISKO model of Bunnell & Dowding (this volume) makes extensive use of both elaborations of the paradigm to handle above- and below-ground decomposition processes. The model attempts to follow the dead vegetation through its numerous phases (standing dead, litter, and humus), and hypothesises the effects of abiotic variables on the decomposition rate of each of these substrates. The model, essentially a dynamic word model acting as a synthesis tool, is driven with data from different tundra sites. The time step in the model is one day.

The general format developed by Jones & Gore (in press), Clymo (in press) and Bunnell & Dowding (this volume) can be used to describe or mimic a very wide range of natural phenomena. In terms of mimicking data, adding an extra box or sub-dividing a box into independent boxes is in some sense analogous to using a higher-order polynomial in regression analysis. The essential difference, however, is that often the extra box can have, or *appear* to have, biological significance.

With increased complexity the model's output not only mimics the data more closely, but the model's construction serves as a more complete description of the system's workings. For example, a litter bag model of the form shown in example 1 is a simple one-compartment representation of decomposition which assumes that on the average the environmental conditions contributing to weight loss are the same from year to year. These assumptions imply that there is an average yearly substrate-specific, site-specific decay rate. In terms of the general paradigm, I for the first iteration (or year) could be the total dry weight of litter placed in a litter bag. The rest of the iterations I would be zero. T for each successive iteration would represent the remaining weight of the litter bag from year to year. A fitting parameter a is derived by regressing log (T) against time. For total litter from Barrow the model works reasonably well.

For substrates other than total litter the assumption of a single substrate-specific, site-specific decay rate is inadequate. The generality that the rate of weight loss gradually declines over time is equally well supported for tundra systems as for other systems (F. Bunnell, 1973; Flanagan & Veum, this volume; Heal & French, this volume). Thus material that is presently less than one year old will have distinctly different decay rates from one year to the next.

An improved fit can be obtained by dividing the substrate into two components which have initial weights W_1 and W_2 and average annual rates of weight loss of r_1 and r_2 respectively. One of the substrate components, say W_1, is assumed to lose weight or "disappear" more rapidly than the other. The component W_1 might represent readily leachable material. Total weight as a function of time, W (t), is then given by

$$W(t) = W_1 e^{-r_1 t} + W_2 e^{-r_2 t} \tag{1}$$

The model of equation 1 is a relatively "soft" or "loose" model since a wide range of values for W_1, W_2, r_1 and r_2 can be used to predict weight losses within the range of observed litter bag losses. In terms of the general paradigm the model consists of two independent compartments. There are three fitting parameters, r_1, r_2, and the proportion of litter going to compartment 1. In this case the extra box appears reasonable, representing a faster moving compound group within the original substrate. Although this is reasonable it should not distract one from an awareness of the arbitrariness of the model. The "fast" compound group must first be chemically defined and measured (Flanagan & Veum, this volume).

The changing rates of weight loss of litter can be mimicked without explicitly simulating changes in chemical composition. One year old litter might be assigned a slower decomposition rate than current or "fresh" litter without relating the slower decomposition rate directly to chemical composition. Or in terms of the paradigm the model would have the form of example 3 but with only one generalized input.

After one year all of the new litter T_1 would be transferred to the one year or older compartment T_2. Single species models of decomposition may employ this approach (Bunnell & Dowding, this volume, and the treatment of individual species by Jones & Gore, in press).

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A large part of the decomposition modeling efforts of the US Tundra Biome has been directed towards removing the arbitrariness of the fitting parameter a in the general litter bag model, or in other words, the efforts have attempted to derive or measure a independently. As the following review of US Tundra Biome modeling will illustrate, these efforts have often introduced more fitting parameters that appear biologically based but these parameters have not been or sometimes cannot be measured.

The first "improvement" over a constant annual decay rate occurred in TCOMP, an ecosystem model by Bunnell (Brown, 1971) described in Miller, Collier & Bunnell (1973). The decay rate was assumed to be a linear function of temperature with the maximal decay rate a function of the age of the substrate. Within TCOMP one year old standing dead decayed faster than two year old standing dead, thereby implicitly incorporating changes in chemical composition. It should be noted that in 1971 there were insufficient respirometry data to test the correlation with temperature easily. The model simply used a value that produced a suitable yearly rate.

The model developed in February 1972 (Bunnell, Bunnell, Oguss & Walters, 1972) attempted to incorporate measurable, biologically meaningful components by dividing decomposition, the phenomenon of weight loss, into two processes: respiration by microorganisms utilizing the substrate, and leaching. Since the model was still ahead of the data (as it should be), both respiration and leaching rates were made simple functions of temperature. Due to the failure of this reworded TCOMP to mimic observed standing dead transients a moisture effect was incorporated in the model. The first mathematical formulation of what was eventually to become GRESP thus postulated respiration rates to be a linear function of temperature reduced by declining moisture levels in a sigmoid fashion.

The new formulation was applied only to the litter compartment. Since no data were available for moisture levels in standing dead vegetatation moisture was assumed to vary inversely with air temperature. This moisture index, ranging from 0 to 1, was used to reduce multiplicatively the computed respiration rate. The increased "realism" in the model's output was without detailed biological substance. While the mathematical representation mimicked biological understanding, each individual parameter in the operation could *not* be ascribed an easily measured biological meaning. For almost a year, the modeling effort with respect to GRESP consisted in "improving" or refining the mimicry while appearing to be adding more biology.

At the meeting of the International Decomposition Working Group in Abisko, Sweden, the respiration rate, as a function of temperature and moisture, was given the general shape indicated in Fig. 1. Moisture levels were assumed to depress respiration rates in a curvilinear fashion at both high and low moisture levels. This hump-shaped curve was assumed to be a general property of microorganisms and therefore applicable to standing dead, litter and soil substrates. In October 1972 researchers within the Decomposition/Nutrient Flux working group of the US Tundra Biome simulated the respiration rate as a hump-shaped function of moisture content and assumed that the moisture level at which the maximum respiration rate occurred increased with increasing temperature. As before, the general height of the respiration curve also increased with increasing temperature. The model thus had the general form implied by observations of Douglas & Tedrow (1959).
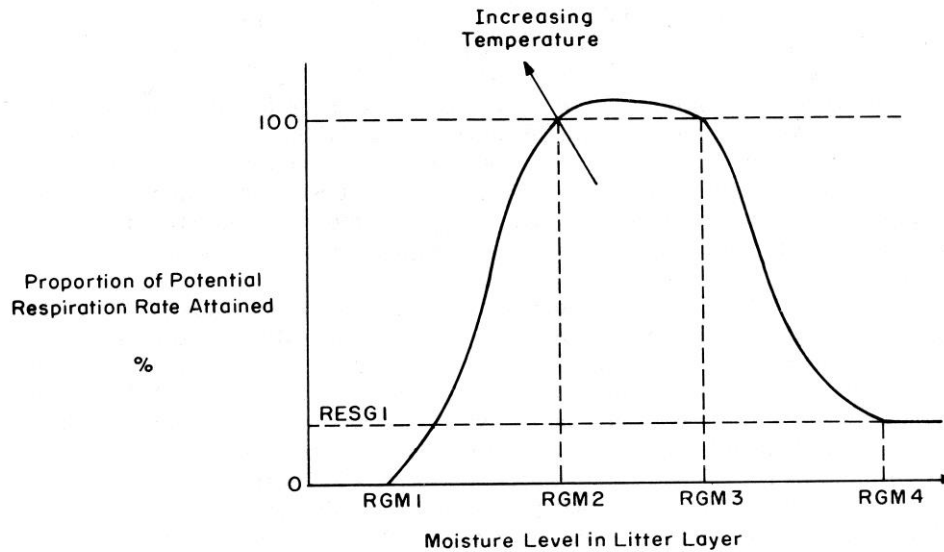
Figure 1. Effect of moisture level on litter respiration rate.

The HUMP or GRESP model of October 1972 is illustrated in Fig. 2. Note that peak respiration rates shift up or to the left in Fig. 1 and up and to the right in Fig. 2. Both formulations are based on empirical evidence; it is still unclear which, if either, formulation is correct. The disparity between these two figures reveals the dangers inherent in modeling to fit data as opposed to fitting theory.
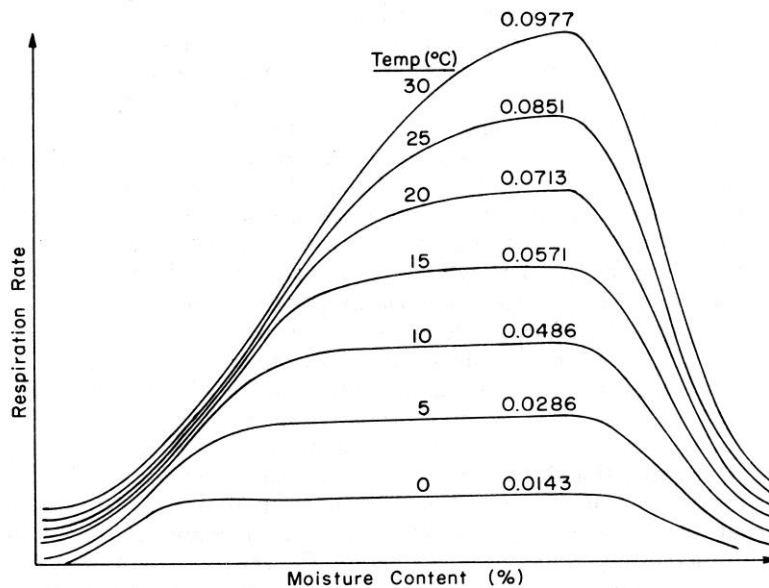

Figure 2. Semi-perspective plot of computed respiration rate at different temperature and moisture levels. All curves actually begin at the origin. (From Tait & Bunnell, 1972.)

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It was during the same October workshop that an attempt was made to incorporate the chemical composition of the decomposing substrate explicitly. DECOMP (Bunnell, Bunnell & Tait, 1972) provided a dynamic framework within which leaching and microbial activity (as represented by substrate respiration rates) could alter the chemical composition which in turn could alter the leaching and respiration rates. The basic ideas followed conceptual expansions similar to those experienced by GRESP. Confronted with insufficient data the number of distinct compound groups arbitrarily started at three, expanded to four and has now been reduced to two.

Acknowledging the experience with conceptual detail obscuring measurable facts, the U.S. program has been less adventurous in its attempts to incorporate microfloral and microfaunal comminution into decomposition modeling. The problem has been superficially incorporated in ABISKO (Bunnell & Dowding, this volume), and attempted in some detail for the Devon Island site (Whitfield, 1973).

In summary and with respect to the general paradigm, it is clear that the simple litter bag model has been greatly elaborated. In the three compound version of DECOMP, a particular substrate such as standing dead has been expanded into nine independent compartments: three canopy heights with three compound groups each. The decay rate parameter a has become three complex hump-shaped functions of temperature and moisture, one for each compound group. The model, as a result, incorporates a large number of fitting parameters to allow it to mimic such things as the poorly known seasonal patterns of chemical composition in the various substrates.

Expressed as a word model of decomposition processes the U.S. tundra models express the following concepts:

1. "Decomposition" is considered to be the process of weight loss from dead material through the mechanisms of respiration and leaching. Comminution by microflora and microfauna is not included, not because it is considered unimportant but because researchers have been unable to separate the effect from other processes in the field. Mineralization of elements other than carbon in the soil is not considered.

2. One can consider the microbial population as a "functional group." As a result one need not consider the microbial population dynamics. Whatever group of organisms becomes established on the substrate will respond to temperature and moisture in much the same fashion. Groups that would respond "inappropriately" are not established. This may or may not be true. As with comminution by microflora and microfauna, until more is known it cannot adequately be modeled.

3. The respiration rates of microorganisms are assumed to increase with temperature but will be limited by too little water or too much water.

IMPLICIT AND EXPLICIT THEORY IN MODELS OF DECOMPOSITION

We have already indicated that simulation models can be used to describe or to mimic a wide range of natural phenomena. Underlying the presentation has been the idea that sometimes "complex" models are nothing more than cleverly disguised "high order polynomials" in the sense that high order polynomials are often good "curve fitters." At other times the models represent biologically feasible constructs or

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guesses and once in a great while the model represents explicit biological theory. The following section will attempt to clarify potential differences between models devised as "curve fitters" and models based on explicit statements of biological theory.

Explicit assumptions and theories are those encoded directly by our mathematical statements or model. Implicit assumptions and theories are those which may have guided our mathematical formulation but are either not encoded in the model or are encoded in an arbitrary fashion as a fitting parameter or a "suitably shaped" function. Modeling and research efforts are primarily directed towards transforming implicit theory into explicit theory. It is interesting to note that the incorporation of explicit theory often does not allow one to simulate natural response patterns as well as analogous models using implicit theory. However, the more explicit the theory that is incorporated, the more easily the theory is evaluated by the model. To state it differently, implicit theory with its arbitrary fitting parameters and functions tends to generate rather loose "pliable" models that can be shaped to fit the available data. Explicit theory forces the model output into a specific well defined pattern that would be recognized as inconsistent with the data when the data depart from the theory.

As an example, consider the two compartment litter bag model described earlier. If one assumes that the first compound group is rapidly leached and thus almost entirely lost from the litter bag after only one year the model becomes somewhat more structured. Figure 3 illustrates the response patterns of two different models of weight loss from standing dead. Both models represent means of simulating the overall decay rate by postulating different responses for two different substrate constituents. They represent the common case where chemical analyses were not performed. The first model (Fig. 3a) employs the theoretical construct that compound W_1, the "fast moving" compound, is leached out of the system within the first year. Parameters of the model are estimated by fitting the "best" straight line through the data points for year 1, 2, 3 and 4, then extrapolating back to time 0 to determine W_2 (note that Fig. 3 represents a semi-log plot). The slope of the "best" straight line represents the decay rate for compound W_2. The remainder of the substrate, W_1, is decayed or leached at a rate r_1, which is indeterminable from litter bag data alone. Within the theoretical construct r_1 need only be large enough to remove almost all of W_1 within one year. If we postulate that after one year the amount of W_1 remaining is no more than 0.5% of the total original weight then r_1 can have any value ≥ 3.9 per year (a loss rate, in this case, of ≥ 0.98 g/g per year).

Fig. 3b depicts the best mathematical fit to equation 1 given no assumptions or theoretical constructs concerning leaching. Compound W_1 is assumed to move faster but need not be entirely removed in the first year. The increased goodness of fit is obtained by first fitting a straight line (exponential decay) through data points for years 2, 3 and 4, thereby estimating W_2 and r_2. Since fewer theoretical constraints are placed on W_1 and r_1 they can be manipulated to fill in the curve over the first two years. In Fig. 3b 8% of the original value of W_1 is still present after one year, but the mathematical fit is closer. In the second, less constrained model r_1 is especially sensitive to very small variations in W_2 and r_2.

One could add further explicit constraints by *operationally* defining the fast compound group on the basis of chemical analysis. This idea of explicit versus implicit constraints is in some sense analogous to the "direct" versus the "indirect" method of Clymo (in press). Clymo's direct estimate consists of utilizing "measured" values of his parameters for production, compression, creep, aerobic decay rate, and anaerobic decay rate. He then compares the model output with age and density versus depth profiles. His indirect approach consists of fitting the model to the depth profiles and estimating the appropriate parameters.
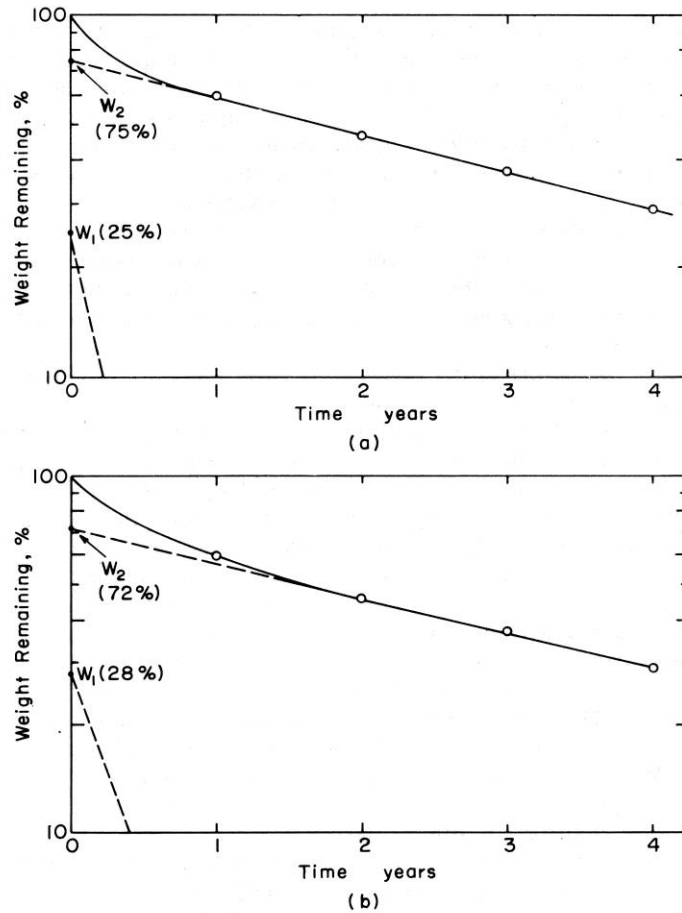
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Figure 3. Weight loss from standing dead: explicit theory versus best mathematical fit in a two compartment model (see text for explanation).

As indicated earlier, the incorporation of respiration rates of decomposer microorganisms was an attempt to replace the arbitrary constant yearly loss rate of the litter bag model with explicit "directly" measurable parameters (measurable at least with respect to a particular environment). In the US Tundra Biome program a number of temperature-moisture-respiration rate response surfaces have been measured in the field and the laboratory for various substrates. Models incorporating functions representing these response surfaces can be integrated over a specific year's temperature and moisture conditions to produce independent estimates of litter bag weight losses.

With the incorporation of this additional explicit theory more refined statements can be made about decomposition dynamics. For example, model structure now permits comparisons from year to year and should help to reveal the manner in which year to year climatic differences influence year to year loss rate. The model also allows one to examine intraseasonal patterns of litter bag weight loss.

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Unfortunately, typical litter bag experiments do not represent critical tests of the models. There are two reasons; one is the nature of the question, the second is the variation inherent in the litter bag data (Heal & French, this volume). The question is not simply "Can we predict average litter bag weight losses from a model based on respiratory responses?" (simpler constant coefficient litter bag models can predict well within the error variance of the data). Rather, the question is "Can a model based on respiratory responses account for the variation in litter bag weight losses between years of different weather conditions?" We are not at this time concerned with changes in substrate quality through time, but with between-year variation for the same substrate. To date there have been no rigorous attempts made to evaluate the relative accuracy of models incorporating respiration responses with simpler constant coefficient models.

Furthermore, the nature of the variation in litter bag data largely eliminates these data as a candidate means for independently evaluating respiration models. The fact that one can reasonably fit a straight line through semi-log plots of litter bag weights against time and is not statistically forced to use line segments or a curve suggests that either there is no variation due to different annual weather patterns or that the data are not restrictive enough to detect this variation. Note that if there is really no difference due to annual weather patterns the fundamental premise in generating such models is violated except for extreme conditions and their primary use is in documenting substrate differences. The data we have examined indicate that the explanation is simpler: within-year variation for litter bag data is often as high as between-year variation. These data will often statistically accommodate a simple negative exponential fit even when the underlying processes almost certainly depart from this pattern. Heal (pers. comm.) has stated that when measured at intervals of less than a year, the pattern of weight loss does depart significantly from a negative exponential. We have been unable to obtain sufficient data of the form described by Heal to evaluate rigorously the accuracy of our models simulating weight loss due to respiration other than on an annual basis.

Models incorporating a functional response to moisture and temperature, such as respiration, can be used to explore the potential effect of different climatic patterns on a particular site-specific substrate. Thus, we should be able to predict litter bag weight losses for total litter from Barrow, Alaska, placed on the site at Glenamoy, Ireland. That extrapolation does not suggest that we can predict litter bag losses for Glenamoy litter at Glenamoy. We would first have to determine the response surface for Glenamoy litter.

Accepting these constraints it is still interesting to explore the potential differences in decomposition at any one site that may be attributable to different microclimates. Since the general pattern of the response surface does seem applicable over a wide variety of substrates, one can ask some broadly applicable questions. For example, what is the influence of diurnal temperature pattern on decomposition?

For the simple case of a constant moisture level we have calculated that a diurnal temperature range of 10°C will increase the total daily respiration by 12% over that computed using average temperature. Data employed in this calculation were those of Flanagan for total litter, responding to temperature with a Q_{10} of 4 (Appendix 1).

The magnitude of the diurnal effect is important for at least two reasons. First, it indicates that extreme care should be taken when attempting to evaluate or extrapolate models that are assumed to be predictive. Second, it indicates the possibility of explaining some of the observed intersite differences in decomposition rates.

We wish to emphasize that the example of the diurnal temperature effect presented is for the simplest case of a constant moisture level. Fig. 1 and 2 illustrate that both temperature and moisture influence respiration rates in a non-linear fashion and that the interaction between temperature and moisture is also non-linear. Before even a simple model such as that illustrated in Fig. 2 is employed as a synthesis or comparative tool, we must be confident about the form of the interaction effect as well as each single influencing factor. We will discuss problems in describing the pattern of interaction effects shortly.

The Explicit Incorporation of Substrate Quality

A critical evaluation of extant decomposition models, notably DECOMP, suggests the following two approaches to explicit incorporation of substrate quality.

The direct method might consist of experimentally determining the decomposition rates of different pure chemical substrates. Some work has already proceeded in this direction (Flanagan & Scarborough, this volume; Rosswall, this volume). It is possible that the decomposer populations may behave in an "abnormal" manner when confronted with these pure and thus "foreign" substrates.

An indirect method for explicitly incorporating substrate quality into DECOMP requires a large number of temperature-moisture-respiration rate response surfaces for a number of different substrates. The model's assumption that the substrate can be subdivided into a number of *independent* broad chemical groups is both elegant and generous. It implies that the total temperature-moisture-respiration response surface is a linear combination of the chemical-specific response surfaces with each chemical-specific response surface contributing in proportion to the amount of that chemical group in the substrate. This assumption does not differ significantly from Minderman's (1968) findings that "Experimental results of decomposition show a curve that corresponds in shape with that constructed by summation of a number of exponential functions."

Stated differently, the theory implies that a linear multiple regression analysis of the combined respiration rates of various substrates at specific temperature-moisture points will generate the chemical-specific, temperature-specific, moisture-specific respiration rates.

$$R(T,M) = b_0(T,M) + b_1(T,M)C_1 + \ldots + b_n(T,M)C_n \qquad (2)$$

where

$R(T,M)$ = the computed overall respiration rate at temperature T and moisture level M,

$b_i(T,M)$ $(i = 0, \ldots, n)$ = regression coefficients assumed equitable with the respiration rate of each chemical compound i at temperature T and moisture level M,

$C_i(i = 1, \ldots, n)$ = the amount of chemical compound i,

(T,M) represents the set of temperature and moisture values necessary to complete the respiration response surface.

Note that the model of equation 2 relates chemical composition explicitly to the response surface for microbial respiration. If the general regression model of equation 2 is examined at sufficient temperature-moisture points a family of chemical-specific response surfaces can be generated. The data requirements for generating the regression model are complete temperature-moisture response surfaces for a number of chemically diverse substrates. The number of different substrates depends to some extent on the number of chemical compounds considered in the model. That is, if we wish to differentially simulate the decomposition of several compound groups, we

need to examine response surfaces of several substrates where these compound groups occur in different proportions. At the time of writing we have sufficient data available to generate the temperature-moisture response surfaces for one substrate type, total litter. A few other response surfaces are nearing the completeness necessary for analysis.

The test of the theory embodied in the regression model as presented in equation 2 is twofold. The first test is whether or not multiple regression can successfully partition the variance or whether covariance is critical. Assuming that independence holds and chemical-specific response surfaces can be generated, the second test is whether or not these surfaces can be used to generate the response transient observed in the general decay rate of the entire substrate. For example, the DECOMP model should be able to generate the chemical composition of two year old standing dead by integrating loss rates over one year for one year old standing dead. Failure of the model to do this would indicate that our basic assumptions concerning substrate quality were probably invalid. The significant difference between this approach and that of Van Cleve (this volume) is the attempt made in equation 2 to include the abiotic influences of temperature and moisture.

There is at least one other intriguing approach to examining chemical-specific response surfaces. This approach incorporates the physiological potential of the active microorganisms and is being pursued in the model MICRO (P. Bunnell, 1973). Given the metabolic response of an organism to a number of variables including temperature and moisture the chemical-specific uptake per gram of organism is computed. As the species composition of the microorganism population shifts in response to changing environments, chemical-specific loss rates from the decomposing substrate are generated.

Implicit and Explicit Constraints on Respiration Models

The development of temperature-moisture-respiration rate response surfaces marked an attempt to estimate or measure explicitly what had previously been implicit theory. These response surfaces, in turn, have generated their own set of implicit assumptions. The implicit theory requires respiration rates to rise and fall in some hump or dome shaped fashion (Fig. 1 and 2). As a result, a number of arbitrarily dome-shaped functions have been fitted to the data.

The following theory is presented as an example of the type of explicit formulation required to explain some of the characteristics presently observed in the data. Stated broadly, respiration or microbial and fungal metabolism is assumed to be a function of the supply rates of water, oxygen and nutrients. The problem thus reduces to investigating how the physical and chemical nature of a generalized substrate affects the supply of each of these necessities to the respiring organisms. As it presently stands the theory applies only to aerobic respiration.

The first factor, water, is required either as an external supply of free water for the organism's metabolism, or as an environmental condition to prevent destruction through desiccation. In the first case the respiration rate is assumed to be regulated by a factor inversely proportional to the moisture tension within the actual substrate. In the second case the respiration rate is assumed to be regulated by the vapor pressure or relative humidity within the substrate. In either case it is assumed that at low moisture levels the relative humidity within the substrate follows a simple saturation curve as a function of moisture content. The moisture tension of the substrate will thus follow the negative natural logarithm of humidity. A saturation curve is used as a

first approximation of the adsorption capacity of the substrate. The actual relationship will depend on a number of variables, in particular the distribution of pores and pore volumes within the substrate. It is possible to generate empirically the appropriate relationship by examining weight gains of dry substrates subjected to controlled vapor pressures of water.

Thus, as water content (our measured variable) decreases below optimum the respiration rate will decline according to either

$$\ln \frac{1}{\dfrac{M}{a_1 + m}} \tag{3}$$

$$\text{or} \quad \frac{M}{a_1 + M} \tag{4}$$

where M is the percent water content (g H_2O/g dry weight) and a_1 is the percent water content at which the substrate is half-saturated with water. Saturation in this case corresponds to the "field capacity" of the substrate. Operationally it represents the weight gain of the substrate exposed to 100% humidity, so that the internal humidity will also have equilibrated to 100%. Preliminary analyses of the data of Flanagan show that the initial response of respiration rates to increased moisture at the lower moisture levels does not depart significantly from a Michaelis-Menten relationship, suggesting that the relationship of equation 4 is more applicable than equation 3.

Note that the Michaelis-Menten relationship may also hold if the underlying assumption is that water or a moisture film is necessary for transport or sustained nutrient supply as distinct from an intrinsic moisture requirement. At low moisture levels, doubling the water content would be expected to double the available moist substrate and thus the interface between microorganism and substrate. The process of continued moisture increment clearly would possess a saturation level and follow a Michaelis-Menten form.

The second factor, oxygen, clearly interacts with moisture levels. Moisture levels may influence either the rates of oxygen diffusion across moisture films or hinder oxygen transport by physically blocking air channels. If diffusion across moisture films is the key determinant of respiration rates we might assume that high moisture levels will decrease the rate of oxygen supply since oxygen must diffuse through a film whose thickness is inversely proportional to moisture content. We know that the rate of oxygen supply will be proportional to $e^{-\tau}$ where τ represents the thickness of the moisture barrier. If we assume τ to be proportional to moisture content the depletion of oxygen by increased moisture can be expressed as

$$e^{-kM+b} \tag{5}$$

where M is again the moisture content as a percent of dry weight, k represents the thickness of film per percent of moisture content and b represents the percent moisture content required to establish a monomolecular film on all surfaces. Equation 5 is inoperative at moisture levels below b since diffusion no longer takes place.

It is perhaps more likely that the rate of oxygen supply is simply a function of the available channels or pore space within the substrate. The theory then assumes that the substrate is relatively porous and that the available oxygen is not a function of the volume of available space but rather of the number of open or incompletely blocked channels. For lack of a better relation at the present time, the proportion of spaces or channels filled with water is also assumed to follow a simple saturation curve (the "external" spaces on litter or standing dead will not be filled even with a large

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amount of water). Thus the proportion of unfilled spaces and therefore the availability of oxygen will have the following formulation:

$$1 - \frac{M}{a_2 + M} = \frac{a_2}{a_2 + M} \tag{6}$$

where M is again moisture content and a_2 represents the "half saturation" level where full saturation corresponds to the soil sciences concept of "maximum retentive capacity." Maximum retentive capacity is the weight gain of the substrate soaked in water. After soaking, all the pores in the substrates are assumed to be filled with water.

The above formulation is explicit but highly suspect since it depends critically on the internal physical geometry of the substrate. However, the underlying hypothesis can be experimentally tested. Oxygen enrichment experiments might increase the respiration rates, but if equation 6 holds the higher oxygen levels would not affect the manner in which moisture limits respiration. Thus, the peak of the hump-shaped curve of Fig. 1 or 2 might be shifted upwards but the moisture level at which the respiration rate was reduced to half its maximum value would be independent of the oxygen concentration.

The same experiments would help demonstrate the potential validity of equation 5. The apparent shift of optimal moisture level with temperature that is expressed in Fig. 1 is also suggested by Flanagan & Veum (this volume) and may be a simple function of the dynamics of oxygen transport across moisture films. At higher temperatures the optimum respiration rate can only be attained by the organism when the thinness of the moisture film permits oxygen diffusion to occur as rapidly as the temperature determined respiration "demands" it. Recall that the diffusion rate will be proportional to $e^{-\tau}$. If oxygen diffusion is the limiting process the net effect on the respiration surface is that peak respiration rates for the higher temperatures will occur at lower moisture contents. Under conditions of oxygen enrichment, oxygen diffusion would be more efficient and any shift of maximum respiration rates towards lower moisture levels would be dampened. Thus if the phenomenon expressed in equation 5 is an important determinant of respiration rates, oxygen enrichment would perhaps raise the general level of respiration but would reduce any trend for the level to be skewed to the left (Fig. 1).

Note that with explicit theory the evaluation of experimental results is enhanced. If the theory of oxygen limitation at high temperatures is correct and equation 5 holds, the optimal moisture range will broaden with oxygen enrichment. If the height changes but the half saturation points for moisture remain fixed, then equation 6 is more likely to be an accurate description of the underlying phenomenon. Changes in height or width of the plateau will also help reveal the manner in which parameter a_1 of equation 4 interacts with b of equation 5 or a_2 of equation 6. Parameter a_1 essentially determines the height of the moisture effect since it represents the half saturation constant for moisture (or nutrient) supply. Parameters a_2 or b, whichever appears to hold, help determine the breadth of the moisture curve since they represent the half saturation or initial saturation levels for oxygen depletion.

Our preliminary examination of the data suggests that the phenomena expressed by equation 6 are more important in oxygen depletion than changes in the diffusion rate. Van Cleve's data do not show the temperature induced shift in optimal moisture level suggested by Flanagan & Veum (this volume) and until further information is available we suggest that respiration models should include an oxygen depletion factor of the form expressed in equation 6.

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The third factor constellation, nutrients, or the chemical composition of the substrate is assumed to determine the nature of the metabolic reactions that can occur. These reactions are assumed to obey a chemical-specific or substrate-specific Q_{10} relationship with temperature. The problem of deducing the influences of chemical composition on respiration rates has been discussed with regard to equation 2. A formal statement of the explicit respiration model for each general substrate is therefore:

$$R(T,M) \;=\; \underbrace{\frac{M}{a_1 + M}}_{\substack{\text{availability of} \\ \text{water}}} \;\times\; \underbrace{\frac{a_2}{a_2 + M}}_{\substack{\text{availability of} \\ \text{oxygen}}} \;\times\; \underbrace{a_3 \times a_4^{\frac{T-10}{10}}}_{\substack{\text{enzymatic response} \\ \text{to temperature}}} \tag{7}$$

where

$R(T,M)$ = respiration rate at temperature T (°C) and moisture level M (g H_2O/g dry weight $\times$ 100%),

a_1 = percent water at half "field capacity,"

a_2 = percent water at half "maximum retentive capacity,"

a_3 = theoretically optimal respiration rate that would occur at 10°C (unlimited by moisture and likely capable of operational definition),

a_4 = temperature Q_{10} value.

Note that the temperature term could be expressed equally well as

$$\frac{a_3}{a_4} \, e^{\frac{\ln a_4 \, T}{10}} \tag{8}$$

Although the respiration response surface expressed by equation 7 still has a number of empirically determined parameters they all embody some biological or physical meaning and thus do not represent simple curve fitting, but are an explicit statement of theory.

A number of points should be emphasized at this juncture. The model of equation 7 refers only to decomposition, or weight loss through aerobic respiration. Much of the information utilized to develop the model was acquired through experiments employing Gilson respirometry. Respiration rates predicted by the model will therefore underestimate the true rates where anaerobic respiration is significant. The model will not fit the data as well as some of the presently available hump-shaped surfaces. Further, the model is limited in its range of applicability. Most respiration measures show that the respiration rate is limited to zero at a positive moisture level. The model has respiration limited to zero only by a zero moisture level. Similarly, the present expression of the model is only applicable over the range of temperatures for which the Q_{10} function is applicable. The computed respiration rate does not decline to zero when temperatures are too high or too low. Each of these limitations can be removed by incorporating the appropriate fitting parameter. Our personal conviction is that we should rigorously explore at least one model to which we can explicitly ascribe theoretical meaning, before generating further complex fitting routines. We believe that the model as it is stated in equation 7 is sufficiently general to apply to standing dead vegetation, litter and soil.

A Return to Fancy

The incorporation of biologically interpretable parameters into our modeling efforts allows the development of a number of interesting testable but fanciful hypotheses. For instance, the more physically reduced and pitted the substrate the smaller will be the "field capacity" and the larger the "retentive capacity." As the substrate ages the respiration hump with respect to moisture should broaden. However, the change in chemical composition with age will tend to mask this effect. If the substrate is an organic soil, the bulk density might be assumed to be a measure of "packing density." The model of equation 7 predicts that in soils of approximately the same chemical composition, the response of respiration to moisture will be higher and narrower when the soil has a higher "packing density." Soils with higher nutrient levels might indicate a respiration response that was higher, but the response over the moisture domain need not be narrower since the oxygen depletion would not necessarily occur at lower moisture levels.

It should be noted that nutrient supply rates as postulated in the model, and likely in nature, are not a simple function of concentration or amounts of nutrient present independent of physical structure. On a purely physical basis, soils with higher bulk densities or denser packing might be expected to have higher nutrient concentrations since a given unit of water would be exposed to more substrate surfaces. Evacuation and resupply of nutrients in solution would then occur more quickly. The model as postulated in equation 7 predicts that such soils would have a higher respiration rate but not necessarily a higher Q_{10} value.

Our preliminary analyses indicate that Q_{10} values as they are usually measured are remarkably similar for several substrate types. Higher absolute respiration rates may be associated with a particular substrate type due to the form of the respiration versus temperature response near zero. That is, the intercept of the respiration versus temperature curve appears to vary more than the slope in the range where Q_{10} values are usually measured.

There is of course a correlation between respiration rates and chemical composition. In part this is encompassed by the verbal expression of the model in the term "rates of nutrient supply." Ethanol-soluble compounds apparently support more rapid respiration rates, but we have not dealt with this phenomenon in the rigorous fashion suggested by equation 2 and have no explicit representation of it. Preliminary examination suggests that at least in above-ground components the entire respiration response surface is raised or lowered by an amount proportional to the percent ethanol-soluble compounds present. More data are needed before a firm statement can be made.

One clear value of equation 7 as a theoretical construct is the manner in which parameter values can be directly related to microbiology. The manner in which each parameter changes with substrate can be postulated in terms of microbial activities. Parameter a_3 is clearly a function of the enzymatic potential of the microbes relative to the chemical composition of the substrate. Diffusion rates help determine nutrient supply rates, thus the solubility of the substrate is important. As contact between surfaces is important for nutrient exchange one might expect the value of a_3 to increase with increasing bulk density. Parameter a_4 represents the Q_{10} rate and thus is directly related to enzyme kinetics. In above-ground substrates we would expect a_1 to increase as aging or comminution takes place or bulk density decreases, since a moisture film is essential to microbial uptake and it takes more water to fill the less closely packed spaces. However, in below-ground substrates where pressures can collapse and pack

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the aging substrate one would expect the opposite effect (a_1 would decrease as bulk density increases). The physical formulation of a_1 permits an initial incorporation of comminution effects in an explicit fashion. Similarly, the nature of the diffusion process and microbial respiration postulates the manner in which the oxygen parameter a_2 would respond to changes in the physical structure of the substrate such as bulk density.

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APPENDIX 1: CALCULATION OF RESPIRATION
FROM DIURNAL TEMPERATURE

Assuming a $Q_{10} = 4$ as the temperature response for a constant moisture level, the respiration rate is given by

$$R(T,M) = R(0,M) \exp\left[\frac{\ln(4)}{10} T\right]$$

where $R(0,M)$ is the respiration rate at $0°C$ and moisture level M. If one assumes that the diurnal pattern for temperature (T) is of the form

$$T = A + \left(\frac{Mx - Mn}{2}\right) \sin\left(\frac{2\Pi t}{24}\right)$$

where A = average temperature,
  Mx = maximum temperature,
  Mn = minimum temperature,
   t = time in hours.

The integrated daily respiration rate DR is then given by

$$DR = \int_0^{2\Pi} R(0,M) \exp\left[\frac{\ln(4)}{10}\left(A + \frac{Mx - Mn}{2} \sin\theta\right)\right] d\theta$$

which by a Taylor expansion is

$$DR = R(0,M) \exp\left[\frac{\ln(4)}{10} A\right] \int_0^{2\Pi} \sum_{n=0}^{\infty} \frac{\left[\frac{\ln(4)}{10}\left(\frac{Mx - Mn}{2}\right)\sin\theta\right]^n}{n!} d\theta.$$

Using only the average respiration rate, the integrated daily respiration DR_a is given by

$$DR_a = \int_0^{2\Pi} R(0,M) \exp\left[\frac{\ln(4)}{10} A\right] d\theta$$

$$= 2\Pi R(0,M) \exp\left[\frac{\ln(4)}{10} A\right].$$

The percent increase in calculated respiration rate using the diurnal temperature fluctuation is given by

$$100\%\left(\frac{DR - DR_a}{DR_a}\right)$$

which is approximately

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$$\frac{100}{2\Pi}\left\{\int_0^{2\Pi}\sum_{n=0}^{\infty}\frac{\left[\frac{\ln(4)}{10}\left(\frac{Mx-Mn}{2}\right)\sin\theta\right]^n}{n!}\,d\theta-2\Pi\right\}$$

$$\simeq\frac{100}{2\Pi}\left\{2\Pi+\frac{\left[\frac{\ln(4)}{10}\left(\frac{Mx-Mn}{2}\right)\right]^2}{2!}\Pi+\frac{\left[\frac{\ln(4)}{10}\left(\frac{Mx-Mn}{2}\right)\right]^4}{4!}\,\frac{3}{4}\Pi-2\Pi\right\}.$$

If $Mx - Mn = 10$ then

$$\frac{\ln(4)}{10}\left(\frac{Mx-Mn}{2}\right)=\frac{\ln(4)}{2}$$

$$\simeq 0.692147$$

so

$$100\%\left(\frac{DR-DR_a}{DR_a}\right)\simeq 100\%\left(\frac{0.693147^2}{4}+\frac{0.693147^4}{64}\right)$$

$$\simeq 12\%.$$